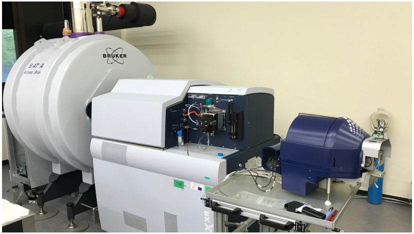
Reconfiguration of graphs with a fixed degree sequence

Nicolas Bousquet, Arnaud Mary

WAOA'18

Mass spectrometry



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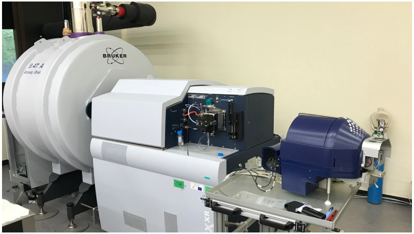

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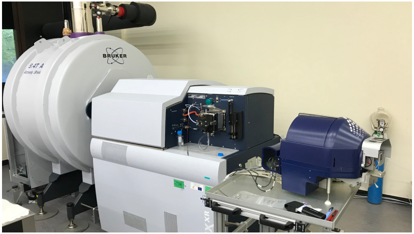

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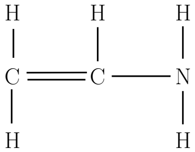
⇒ 

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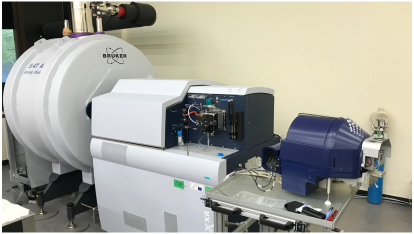

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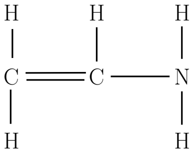
$\Rightarrow$ 

Molecule = Connected loopless multigraph where

Vertices = Atoms.

Vertex degree = Number of bounds.

Realizing a degree sequence

Mathematical formulation :

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Theorem ([Senior '51])

Let $S = d_1, \ldots, d_n$ be a non-increasing degree sequence. There exists a connected loop-free multigraph G with degree sequence S iff :

- $\sum d_i$ is even
- $d_n > 0$
- $\sum d_i \geq 2(n-1)$
- $d_1 \leq \sum_{i=2}^{n} d_i$.

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Question :

Is it necessarily the correct molecule ? $\Rightarrow$ NO !

Structural isomers

Two molecules can have the same degree sequence, they are called (structural) isomers.

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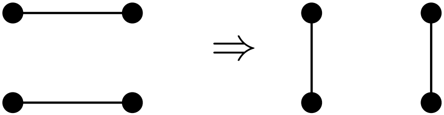
Generation from a seed :

- We start from a graph G with a fixed degree sequence
- We apply an operation that maintains the degree sequence.
- Generation of all the graphs of that DS by repeating this operation ?

The natural operation : flip



Reconfiguration graph

Given a degree sequence S, $\mathcal{G}(S)$ is the graph where

- Vertices = loopless multigraphs with degree sequence S.
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Restriction of the reconfiguration graph :
Given a property Π, we denote by $\mathcal{G}(S, \Pi)$ the induced subgraph of $\mathcal{G}(S)$ restricted to graphs with property Π.

Classical properties Π : Connected, being simple...etc...

Existing results

- Find a graph with a fixed degree sequence S if it exists ?
- Generate all the graphs of degree sequence S using flips ?
- Given two graphs can we find a shortest transformation ?
- Given two graphs can we approximate a shortest transformation ?

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Multigraphs

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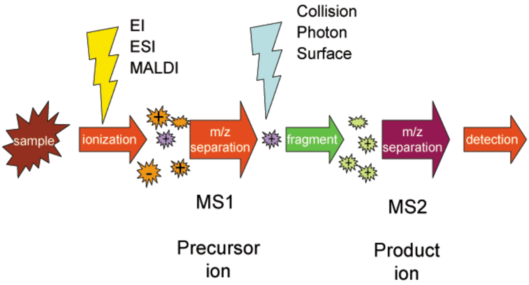
Multigraphs Connected multigraphs.

Tandem mass spectrometry

Figure : wikipedia.com

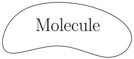
Tandem mass spectrometry



- The molecule is broken into pieces...
- ... which is in turn again broken into pieces...etc...

Figure : wikipedia.com

Tree of the fragments



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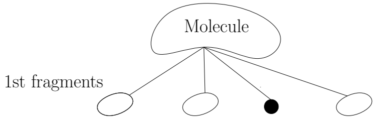

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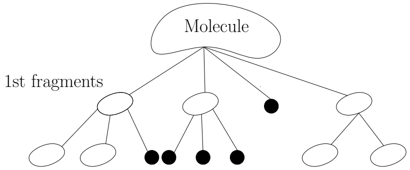

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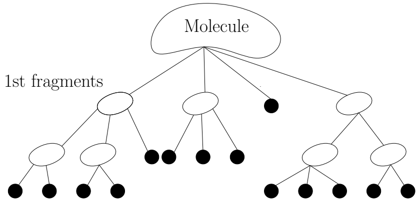

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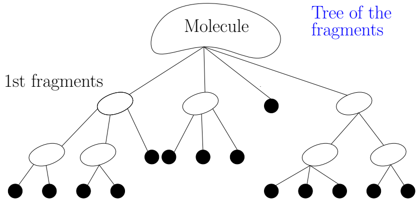

Tree of the fragments :

- Each leaf is an atom $\rightarrow$ its degree is known.

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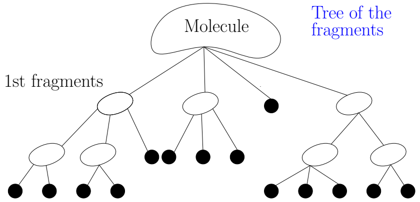

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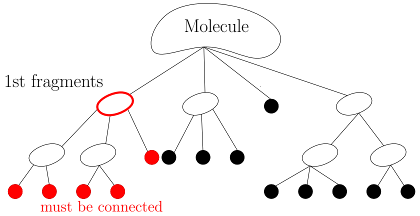

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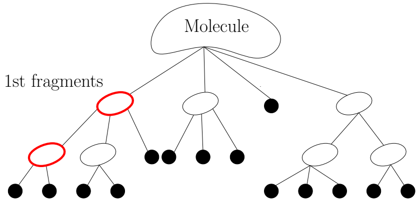

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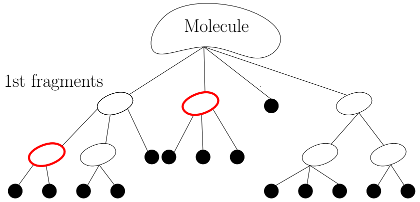

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Combinatorial reformulation

A degree sequence S.
A set of fragments $\mathcal{C}$ that

- contains V
- is nested.

Our property Π :
For every $C \in \mathcal{C}$, $G[C]$ is connected.

$\mathcal{G}(S, \Pi)$: graphs of $\mathcal{G}(S)$ such that every set in $\mathcal{C}$ induces a connected subgraph.

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Questions : Can we still :

- Find a graph that realizes this degree sequence S where each set of $\mathcal{C}$ is connected ?
  $\Leftrightarrow$ Find a graph in $\mathcal{G}(S,\Pi)$?
- Generate all the solutions using flips ?
  $\Leftarrow$ Is $\mathcal{G}(S,\Pi)$ connected ?

Our results

Theorem (B., Mary)

We can find in polynomial time a graph in $\mathcal{G}(S, \Pi)$ if it exists.

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The proof is algorithmic and we can moreover prove the following :

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Given G_1, G_2 in $\mathcal{G}(S, \Pi)$, we can find in polynomial time a transformation from G_1 to G_2 of length at most $(8d + 4) \cdot OPT$.

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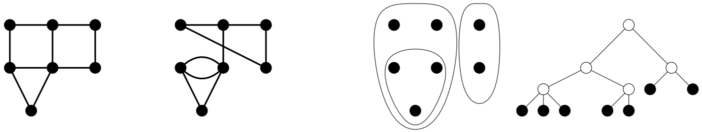
Corollary :

There is a polynomial delay algorithm to enumerate all the graphs in $\mathcal{G}(S, \Pi)$.

Tree augmentation



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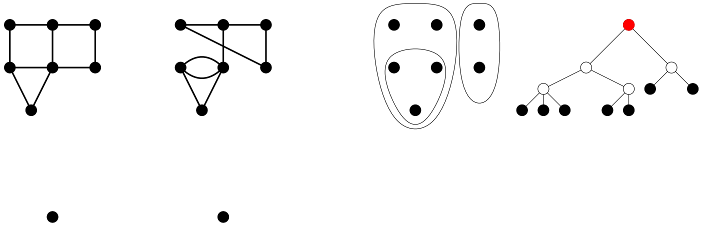

- Start from the root of the tree of the fragments.
- Auxiliary graph : all the fragments that are leaves of the current tree are contracted.

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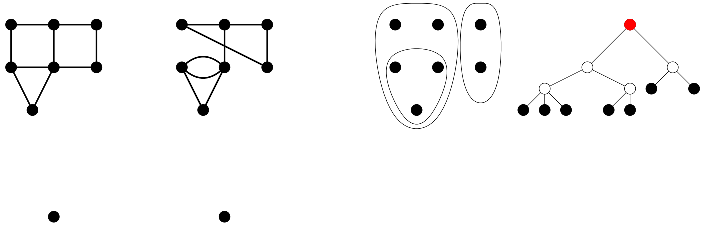

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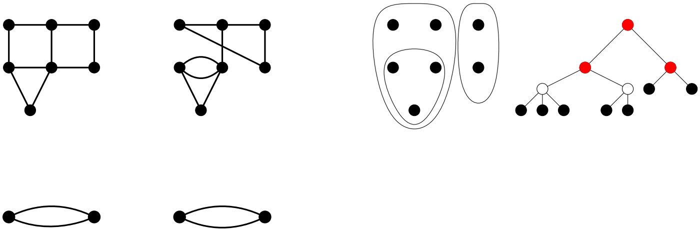

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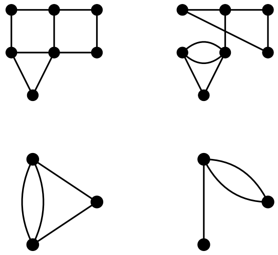

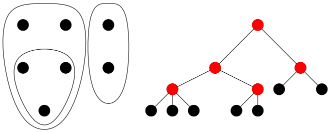

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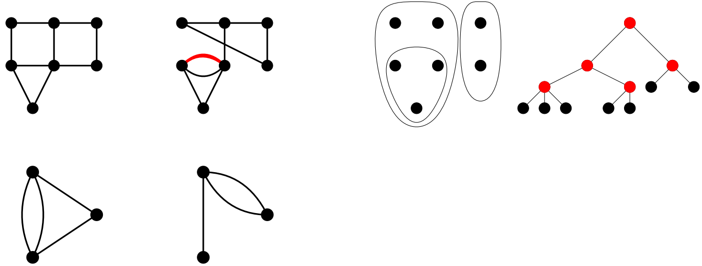

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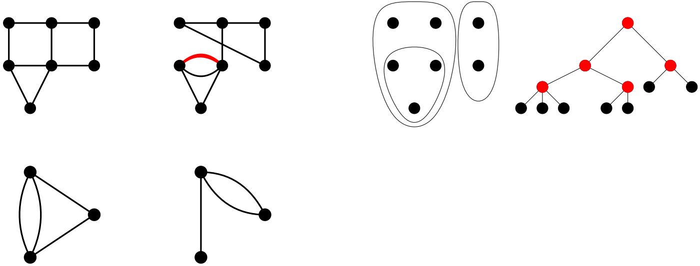

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Sketch :

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semi false...

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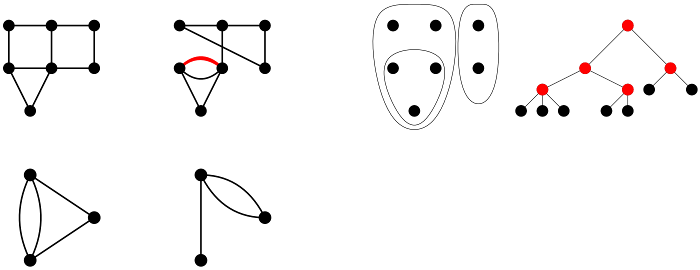

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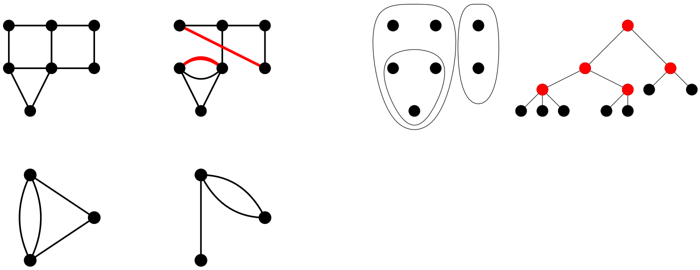

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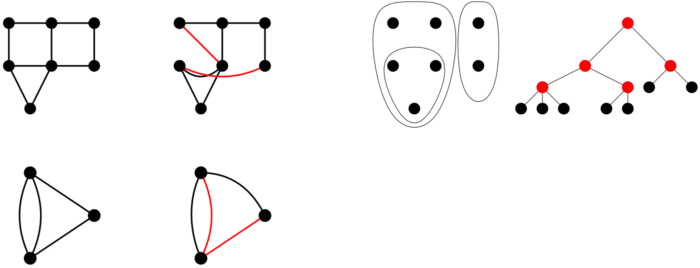

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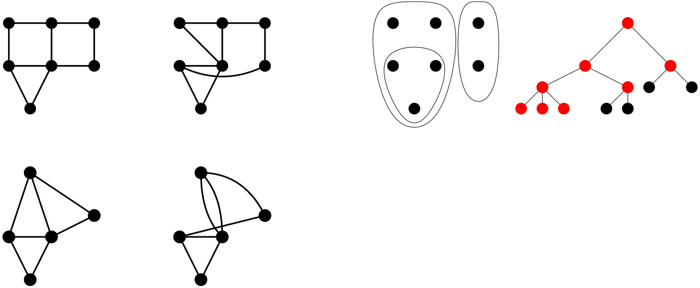

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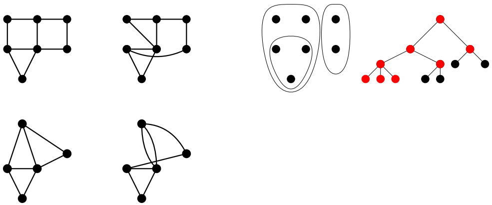

Theorem ([Taylor] [B., Mary])

It is possible to transform the first reduced graph into the second maintaining connectivity.

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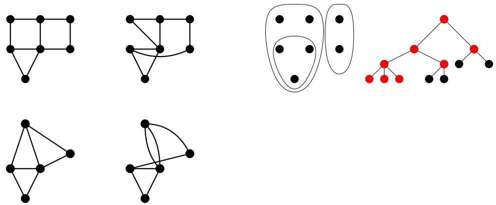

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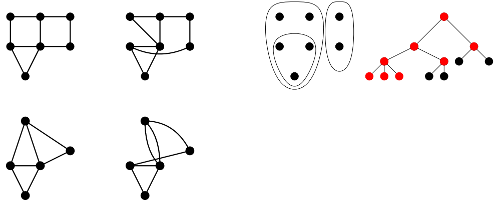

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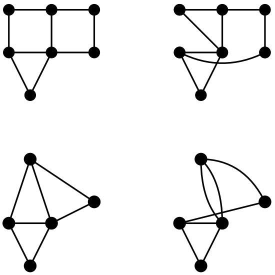
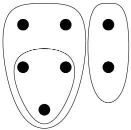
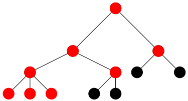
Since the graphs agree before the "extension", the difference is "reduced" to the new set of vertices.

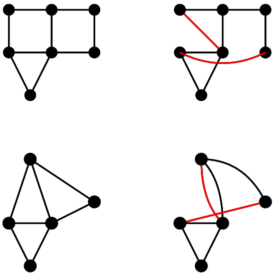
⇒ Only modify edges incident to new vertices.

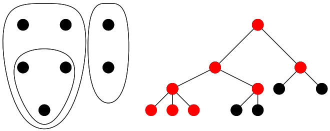
⇒ To ensure it, we define a (new !) auxiliary graph.

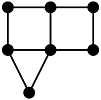


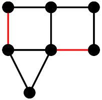


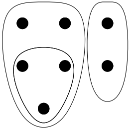


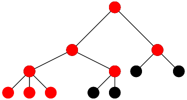


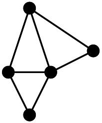


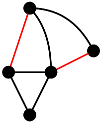


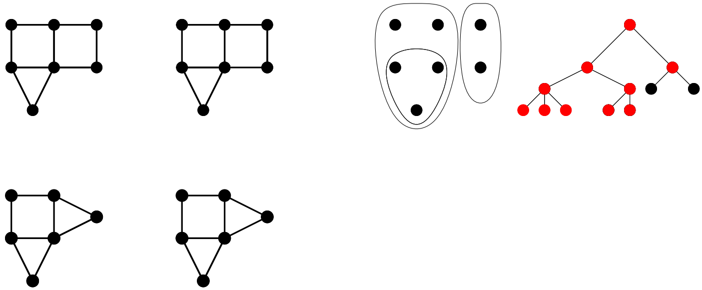




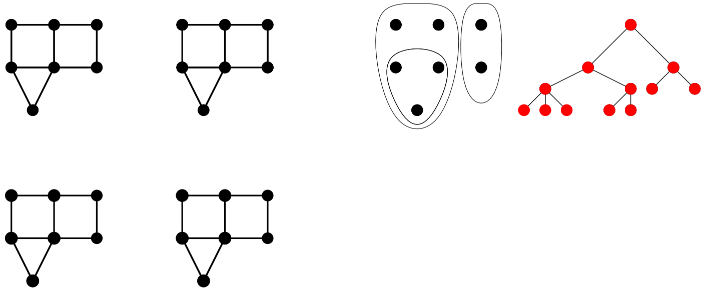








Current tree = Whole tree of the fragments ⇒ the graphs are the same.



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Approximation ratio

Claim 1

We never flip a good edge (an edge of both graphs).

Claim 2

An edge of the symmetric is used at most once to equilibrate degrees.

Claim 3

An edge is modified only when one of its endpoints is “extended” in the tree.

$\Rightarrow$ $(8d + 4)$-approximation algorithm.

Conclusion

- Improve the approximation factor. Can we eliminate the factor depending of the height ?

Conclusion

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Thanks for your attention